Машинное обучение и статистическая физика

Лев Николаевич Щур

Профессор,

заведующий лабораторией вычислительной физики

Семинар «Высокопроизводительные вычисления», НИУ ВШЭ – 12/11/24

Модель памяти Хопфилда и не только

28-я конференция по Статистической физике, университет Токио, август 2024
Профессор Лючилла де Аркангелис, председатель комиссии по Статистической физике IUPAP
вручает медаль Больцмана Джону Хопфилду и Дипаку Дхару.

Формула достижения Хопфилда:
«Расширение границ статистической физики для охвата явлений жизни,
от кинетической коррекции при передаче информации на молекулярном уровне
до динамики нейронных сетей, создание нового языка для осмысления вычислений в мозге»

Нобелевская премия по физике 2024

Формула достижения Хопфилда и Хинтона:
«**за фундаментальные открытия и изобретения, обеспечивающие машинное обучение с помощью искусственных нейронных сетей**»

Первая работа Хопфилда на тему (почти 30 000 ссылок)

Proc. Natl. Acad. Sci. USA
Vol. 79, pp. 2554–2558, April 1982
Biophysics

Neural networks and physical systems with emergent collective computational abilities

(associative memory/parallel processing/categorization/content-addressable memory/fail-soft devices)

J. J. Hopfield

Division of Chemistry and Biology, California Institute of Technology, Pasadena, California 91125; and Bell Laboratories, Murray Hill, New Jersey 07974

Contributed by John J. Hopfield, January 15, 1982

Модель памяти Хопфилда и …

Нейронная сеть Хопфилда (или ассоциативная память) - это разновидность рекуррентной нейронной сети на основе модели спинового стекла, которая может служить в качестве памяти с возможностью контентной адресации.

VOLUME 55, NUMBER 14 PHYSICAL REVIEW LETTERS 30 SEPTEMBER 1985

Storing Infinite Numbers of Patterns in a Spin-Glass Model of Neural Networks

Daniel J. Amit and Hanoch Gutfreund
Racah Institute of Physics, Hebrew University, Jerusalem 91904, Israel

and

H. Sompolinsky
Department of Physics, Bar Ilan University, Ramat Gan, Israel
(Received 11 July 1985)

The Hopfield model for a neural network is studied in the limit when the number p of stored patterns increases with the size N of the network, as $p = \alpha N$. It is shown that, despite its spin-glass features, the model exhibits associative memory for $\alpha < \alpha_c$, $\alpha_c \gtrsim 0.14$. This is a result of the existence at low temperature of $2p$ dynamically stable degenerate states, each of which is almost fully correlated with one of the patterns. These states become ground states at $\alpha < 0.05$. The phase diagram of this rich spin-glass is described.

Модель памяти Хопфилда и …

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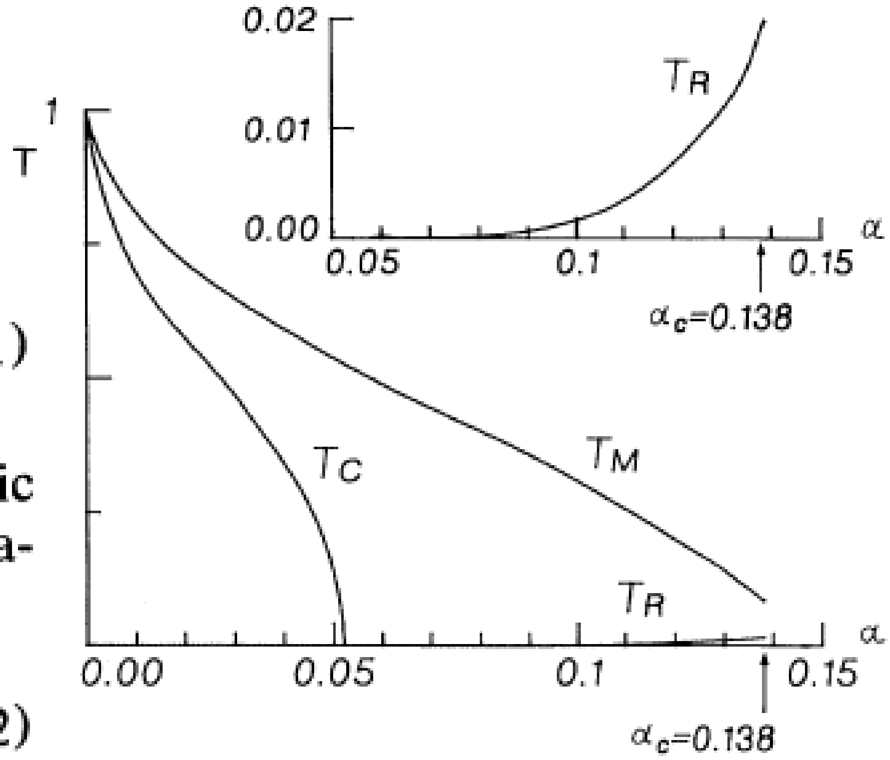
$$H=-\frac{1}{2}\sum_{i\neq j} J_{ij}S_iS_j \tag{1}$$

at temperature $T\,(=\beta^{-1})$. The couplings (synaptic efficiencies) are constructed of p given spin configurations (patterns), according to

$$J_{ij}=\frac{1}{N}\sum_{\mu=1}^{p}\xi_i^{\mu}\xi_j^{\mu}, \tag{2}$$



Plots of critical temperatures of the FM states as a function of α. T_M is the temperature at which FM states first appear. T_c is the first-order transition at which these states become global minima. Replica-symmetry breaking occurs below T_R, which is displayed on an expanded scale in the inset.

Монте-Карло моделирование

Модель памяти Хопфилда и …

EUROPHYSICS LETTERS 15 February 1986

Europhys. Lett., **1** (4), pp. 197-201 (1986)

The Statistical Properties of the Hopfield Model of Memory.

M. V. FEIGELMAN and L. B. IOFFE

Landau Institute for Theoretical Physics - Moscow

(received 26 June 1985, accepted in final form 17 December 1985)

PACS. 75.50K. – Amorphous magnetic materials.

Abstract. – Statistical properties of the Hopfield model of content addressable memory are considered. It is shown that in large systems «phase transition» between regions of «well-functioning» and «chaotic» memory occurs. The phase diagram on the plane (γ, T) is found (γ is the relative number of stored prototype neuron configurations, T is the temperature, *i.e.* the noise intensity).

Модель памяти Хопфилда и …

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$$H = \sum_i V(\sigma_i) - \frac{1}{2}\sum \mathcal{J}_{ij}\sigma_j\sigma_i$$

$$\mathcal{J}_{ij} = \frac{1}{N}\sum_{\lambda=1}^{K} m_i^{(\lambda)} m_j^{(\lambda)}$$

In conclusion, our main results are

a) the transition from the well-functioning memory regime to the chaotic regime is sharp, it occurs at a definite ratio γ of a number of prototype states to the whole number of elements;

b) the critical value of γ tends to zero if $T \to 0$, *i.e.* the effective system constructed on the symmetric Hopfield model needs external noise; it is very interesting if this conclusion holds also for nonsymmetric models of memory.

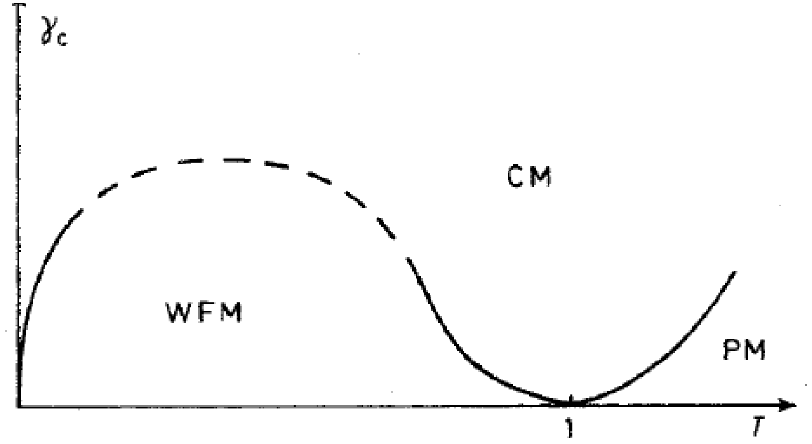

Fig. 1. – The phase diagram of the Hopfield model: WFM denotes the region of the well-functioning memory, CM the «chaotic» memory, PM the paramagnetic phase.

$$F = N\left\{\frac{\tau}{2}\sum_{S,a}(q_a^S)^2 + \frac{1}{12}\sum_{S,S',a}(q_a^S)^2(q_a^{S'})^2(3-2\delta_{SS'}) + \sum_{a>b}\left[Q^{ab}\sum_S q_a^S q_b^S + \frac{1}{2}(Q^{ab})^2\right]\right\}$$

Модель памяти Хопфилда и …

EUROPHYSICS LETTERS 15 February 1986
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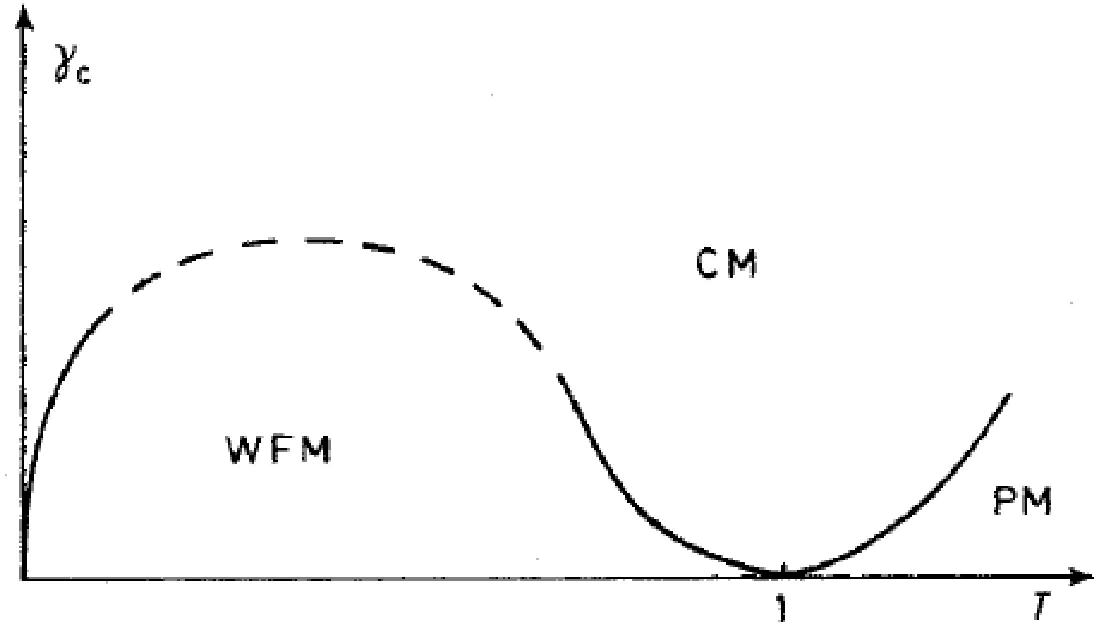

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PHYSICAL REVIEW LETTERS **132,** 077301 (2024)

Editors' Suggestion

Exponential Capacity of Dense Associative Memories

Carlo Lucibello[*] and Marc Mézard[†]

Department of Computing Sciences, Bocconi University, Milano 20136, Italy
and Bocconi Institute for Data Science and Analytics (BIDSA), Milano 20136, Italy

(Received 26 July 2023; revised 29 November 2023; accepted 11 January 2024; published 13 February 2024)

Recent generalizations of the Hopfield model of associative memories are able to store a number P of random patterns that grows exponentially with the number N of neurons, $P = \exp(\alpha N)$. Besides the huge storage capacity, another interesting feature of these networks is their connection to the attention mechanism which is part of the Transformer architecture widely applied in deep learning. In this work, we study a generic family of pattern ensembles using a statistical mechanics analysis which gives exact asymptotic thresholds for the retrieval of a typical pattern, α_1, and lower bounds for the maximum of the load α for which all patterns can be retrieved, α_c, as well as sizes of attraction basins. We discuss in detail the cases of Gaussian and spherical patterns, and show that they display rich and qualitatively different phase diagrams.

REVIEWS OF MODERN PHYSICS, VOLUME 95, JULY–SEPTEMBER 2023

Nobel Lecture: Multiple equilibria*

Giorgio Parisi†

Dipartimento di Fisica, Università di Roma La Sapienza, INFN, Sezione di Roma I, CNR-NANOTEC UOS Roma Piazzale Aldo Moro 2, I-00185 Roma, Italy

(published 17 August 2023)

This is an extended version of my Nobel Lecture, delivered on December 8, 2021. I will recall the genesis of the concept of multiple equilibria in natural sciences. I will then describe my contribution to the development of this concept in the framework of statistical mechanics. Finally, I will briefly mention the cornucopia of applications of these ideas both in physics and in other disciplines.

Нобелевская премия по физике 2021

Формула достижения Паризи:

«**for the discovery of the interplay of disorder and fluctuations in physical systems from atomic to planetary scales**»

Машина Больцмана и протеины …

Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition
Washington, D. C., June, 1983

OPTIMAL PERCEPTUAL INFERENCE

Geoffrey E. Hinton
Computer Science Department
Carnegie-Mellon University

Terrence J. Sejnowski
Biophysics Department
The Johns Hopkins University

COGNITIVE SCIENCE 9, 147–169 (1985)

A Learning Algorithm for Boltzmann Machines*

DAVID H. ACKLEY
GEOFFREY E. HINTON
Computer Science Department
Carnegie-Mellon University
TERRENCE J. SEJNOWSKI
Biophysics Department
The Johns Hopkins University

Машина Больцмана - это сеть симметрично соединенных нейронов, которые принимают стохастические решения о том, быть им включенными или выключенными. Больцмановские машины имеют простой алгоритм обучения (Hinton & Sejnowski, 1983), который позволяет им обнаруживать интересные особенности, представляющие сложные закономерности в обучающих данных.

Нобелевская премия по химии, 2024

½ - Давид Бекер за вычислительный дизайн белков. Он научился осваивать строительные блоки жизни и создавать совершенно новые белки.

½ - Демис Хассабис и Джон Джампер за предсказания структуры белков. Они успешно использовали искусственный интеллект для предсказания структуры почти всех известных белков

Методология, которую мы использовали при разработке AlphaFold, представляет собой сочетание биоинформатики и физического подхода: мы используем физический и геометрический индуктивный подход для создания компонентов.

Highly accurate protein structure prediction with AlphaFold

https://doi.org/10.1038/s41586-021-03819-2

Received: 11 May 2021

Accepted: 12 July 2021

Published online: 15 July 2021

Open access

John Jumper[1,4✉], Richard Evans[1,4], Alexander Pritzel[1,4], Tim Green[1,4], Michael Figurnov[1,4], Olaf Ronneberger[1,4], Kathryn Tunyasuvunakool[1,4], Russ Bates[1,4], Augustin Žídek[1,4], Anna Potapenko[1,4], Alex Bridgland[1,4], Clemens Meyer[1,4], Simon A. A. Kohl[1,4], Andrew J. Ballard[1,4], Andrew Cowie[1,4], Bernardino Romera-Paredes[1,4], Stanislav Nikolov[1,4], Rishub Jain[1,4], Jonas Adler[1], Trevor Back[1], Stig Petersen[1], David Reiman[1], Ellen Clancy[1], Michal Zielinski[1], Martin Steinegger[2,3], Michalina Pacholska[1], Tamas Berghammer[1], Sebastian Bodenstein[1], David Silver[1], Oriol Vinyals[1], Andrew W. Senior[1], Koray Kavukcuoglu[1], Pushmeet Kohli[1] & Demis Hassabis[1,4✉]

RoseTTAFold позволяет решать сложные задачи рентгеновской кристаллографии и крио-ЭМ моделирования, дает представление о функциях белков в отсутствие экспериментально определенных структур и быстро создает точные модели белок-белковых комплексов.

Baek *et al.*, *Science* **373**, 871–876 (2021)   20 August 2021

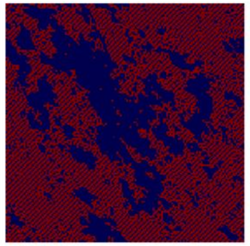
PROTEIN FOLDING

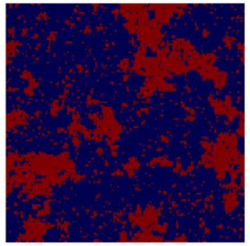
Accurate prediction of protein structures and interactions using a three-track neural network

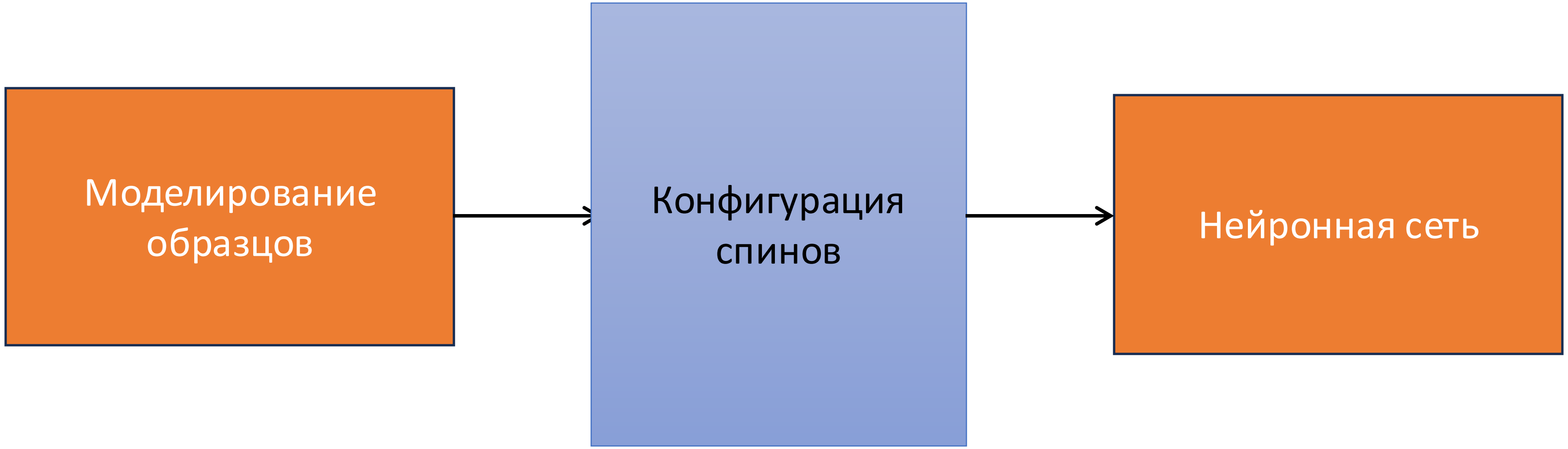
Minkyung Baek[1,2], Frank DiMaio[1,2], Ivan Anishchenko[1,2], Justas Dauparas[1,2], Sergey Ovchinnikov[3,4], Gyu Rie Lee[1,2], Jue Wang[1,2], Qian Cong[5,6], Lisa N. Kinch[7], R. Dustin Schaeffer[6], Claudia Millán[8], Hahnbeom Park[1,2], Carson Adams[1,2], Caleb R. Glassman[9,10,11], Andy DeGiovanni[12], Jose H. Pereira[12], Andria V. Rodrigues[12], Alberdina A. van Dijk[13], Ana C. Ebrecht[13], Diederik J. Opperman[14], Theo Sagmeister[15], Christoph Buhlheller[15,16], Tea Pavkov-Keller[15,17], Manoj K. Rathinaswamy[18], Udit Dalwadi[19], Calvin K. Yip[19], John E. Burke[18], K. Christopher Garcia[9,10,11,20], Nick V. Grishin[6,7,21], Paul D. Adams[12,22], Randy J. Read[8], David Baker[1,2,23]*

Выше: от статфизики к нейронным сетям
Далее: от нейронных сетей к статфизике

- Обучение с учителем – показываем нейронной сети (НН) решетку со спинами (снимок), добавляя признак принадлежности к ферро- (FM) или пара-магнитной (PM) фазе.







Бинарная классификация

- Тестирование – предсказание того, что снимок(T) принадлежит FM фазе. Повторяя много раз получаем вероятность P(T) принадлежности снимков(T) FM фазе.

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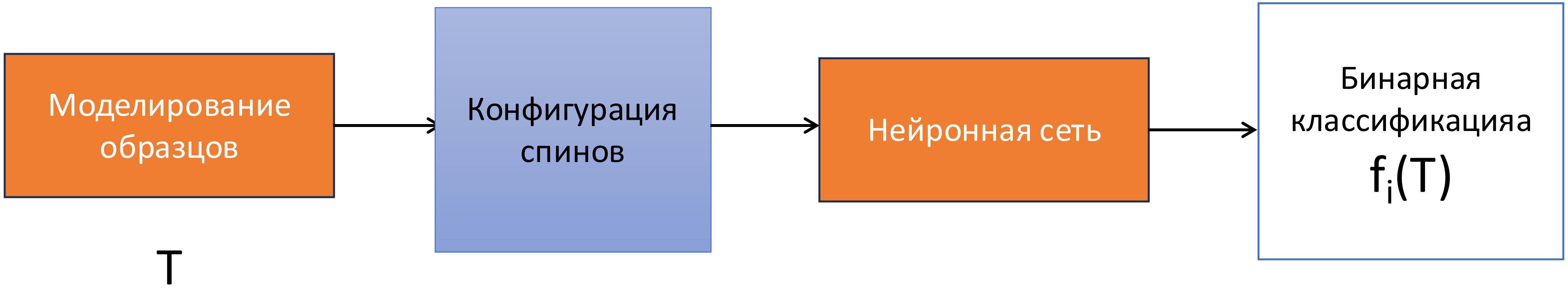
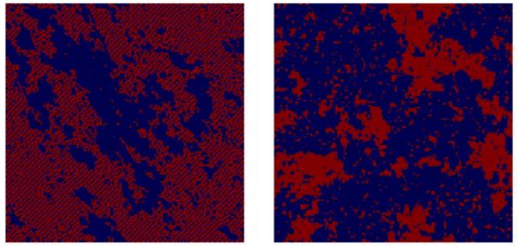
Тестирование

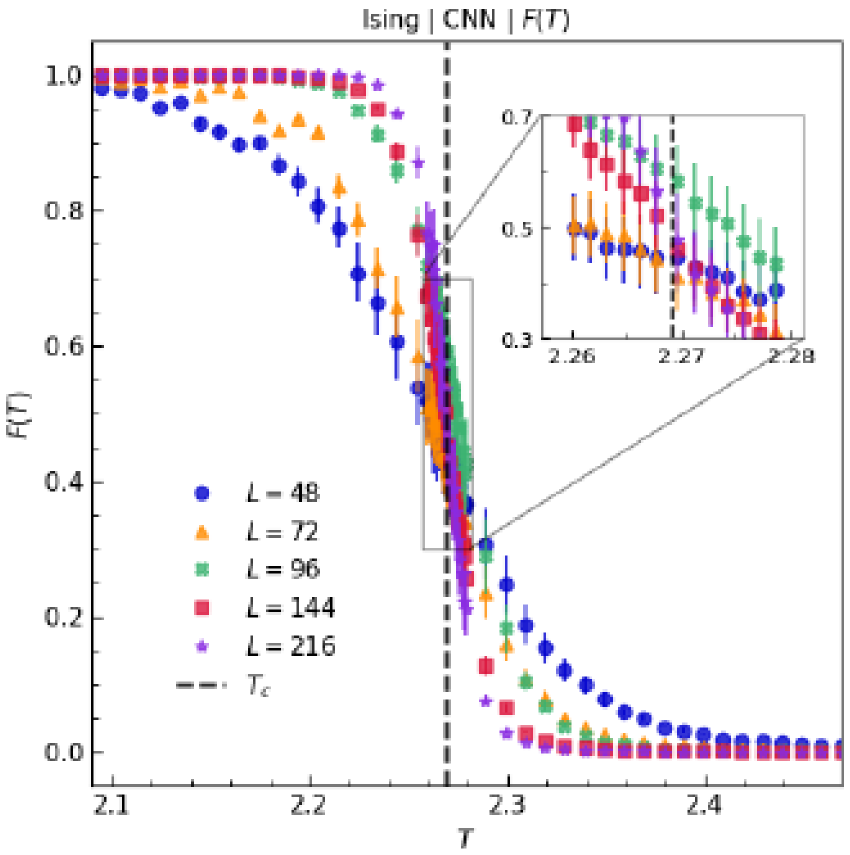


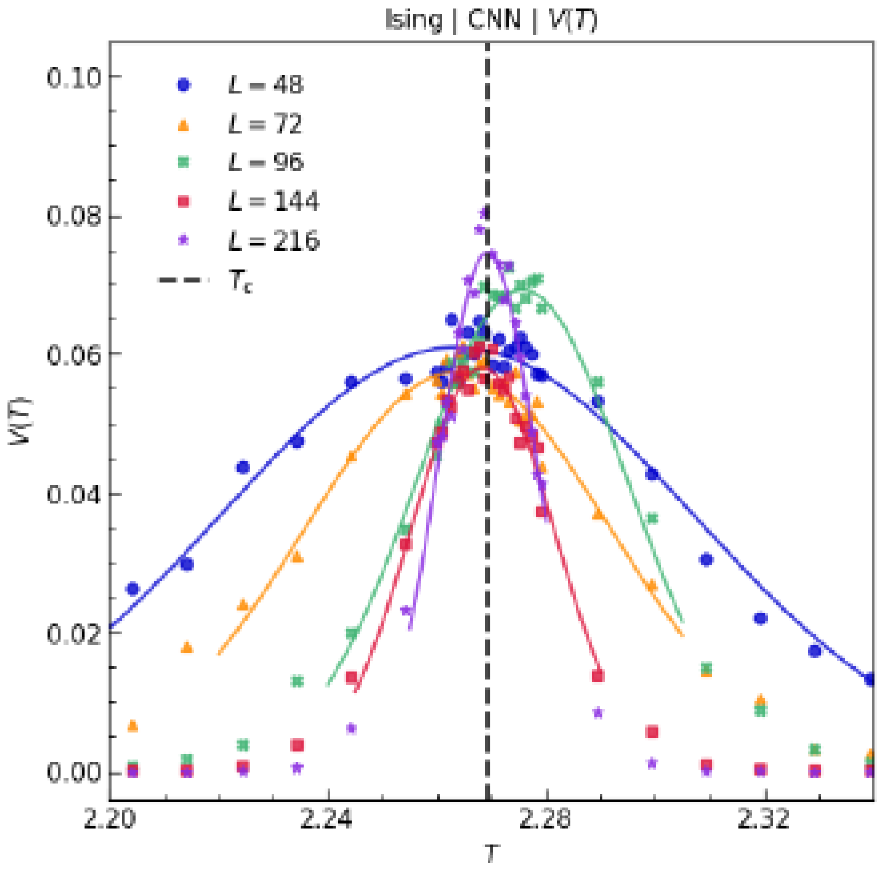


$$P(T;L) = \frac{1}{N}\sum_{i=1}^{N} f_i(T;L)$$

$$P(T;L) = \frac{1}{N}\sum_{i=1}^{N} f_i(T;L)$$

$$V(T;L) = \frac{1}{N}\sum_{i=1}^{N} (f_i(T;L))^2 - (P(T;L))^2$$

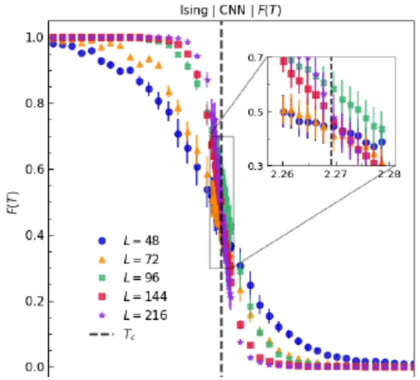




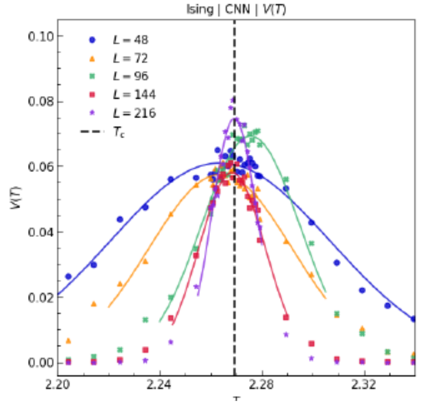
Ширина вариации вероятности V(T)!

$$P(T;L) = \frac{1}{N}\sum_{i=1}^{N} f_i(T;L)$$

$$V(T;L) = \frac{1}{N}\sum_{i=1}^{N} (f_i(T;L))^2 - (P(T;L))^2$$



Ising



NN	$T*$	Δ/σ_T
FCNN	2.2699(5)	1
CNN	2.2727(6)	5
ResNet-10	2.2667(6)	4.2
ResNet-18	2.2688(6)	0.7
ResNet-34	2.2659(6)	5.5
ResNet-50	-	-

$$\mu(L) - T_c \propto 1/L^{1/\nu}$$

$$\sigma(L) \propto 1/L^{1/\nu}$$

Fisher, Ferdinand: PRL (1967)

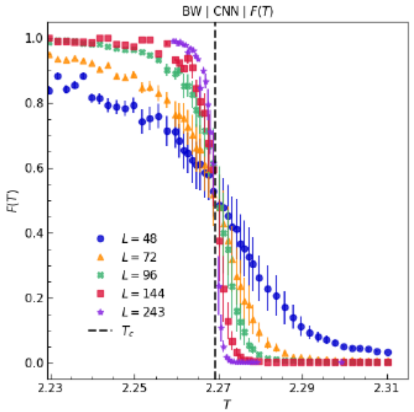
NN	$1/\nu_\sigma$	$1/\nu_{\sigma-}$	$1/\nu_{\sigma+}$
FCNN	1.01(1)	1.02(13)	0.98(4)
CNN	1.06(3)	1.11(5)	1.07(2)
ResNet-10	1.25(3)	1.24(7)	1.24(3)
ResNet-18	1.17(11)	1.41(6)	1.08(10)
ResNet-34	1.15(16)	1.26(7)	1.12(24)
ResNet-50	1.20(5)	1.21(5)	1.31(6)

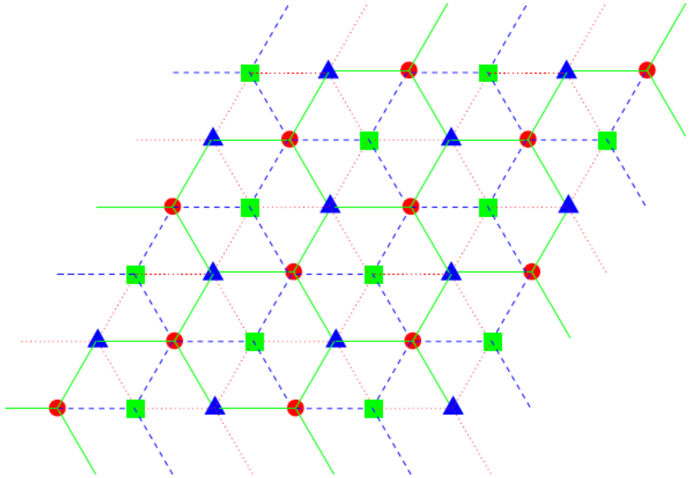
Chertenkov, Burovski, LS: PRE 108 L032102 (2023)

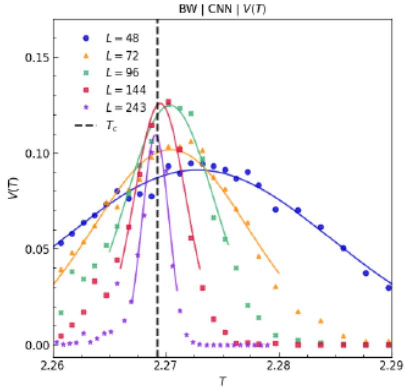
$$P(T;L) = \frac{1}{N}\sum_{i=1}^{N} f_i(T;L)$$

$$V(T;L) = \frac{1}{N}\sum_{i=1}^{N} (f_i(T;L))^2 - (P(T;L))^2$$

Baxter-Wu



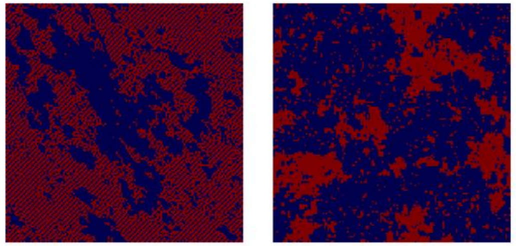




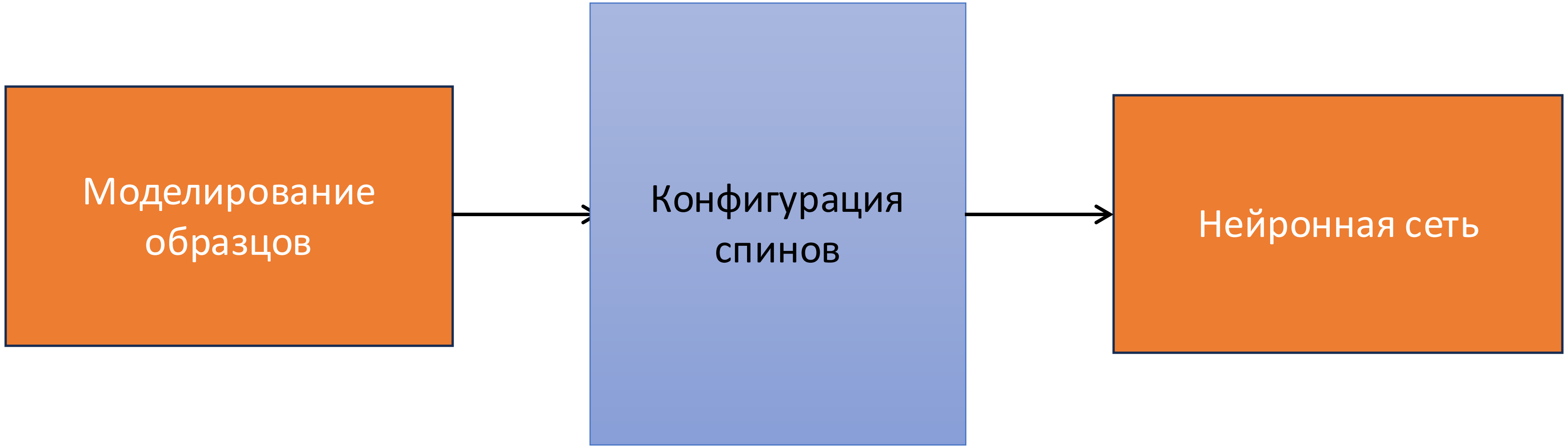
NN	$T*$	Δ/σ_T
FCNN	2.2691(4)	0
CNN	2.2687(4)	1.25
ResNet-10	2.2690(4)	0.25
ResNet-18	2.2684(4)	2
ResNet-34	2.2694(4)	0.5
ResNet-50	2.2688(4)	1

NN	$1/\nu_\sigma$	$1/\nu_{\sigma^-}$	$1/\nu_{\sigma^+}$
FCNN	1.49(3)	1.57(2)	1.38(8)
CNN	1.45(5)	1.55(6)	1.49(5)
ResNet-10	1.48(5)	1.65(13)	1.47(4)
ResNet-18	1.32(11)	1.36(14)	1.40(7)
ResNet-34	1.54(6)	1.76(5)	1.47(3)
ResNet-50	1.43(9)	1.69(16)	1.47(5)

Chertenkov, Burovski, LS: PRE 108 L032102 (2023)



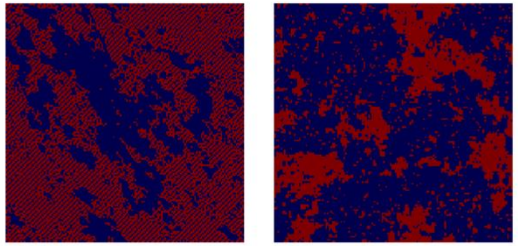
Обучение на изотропной модели



FM/PM

Бинарная классификация

Transfer learning = cross-testing



Тестирование другой модели на обученной сети

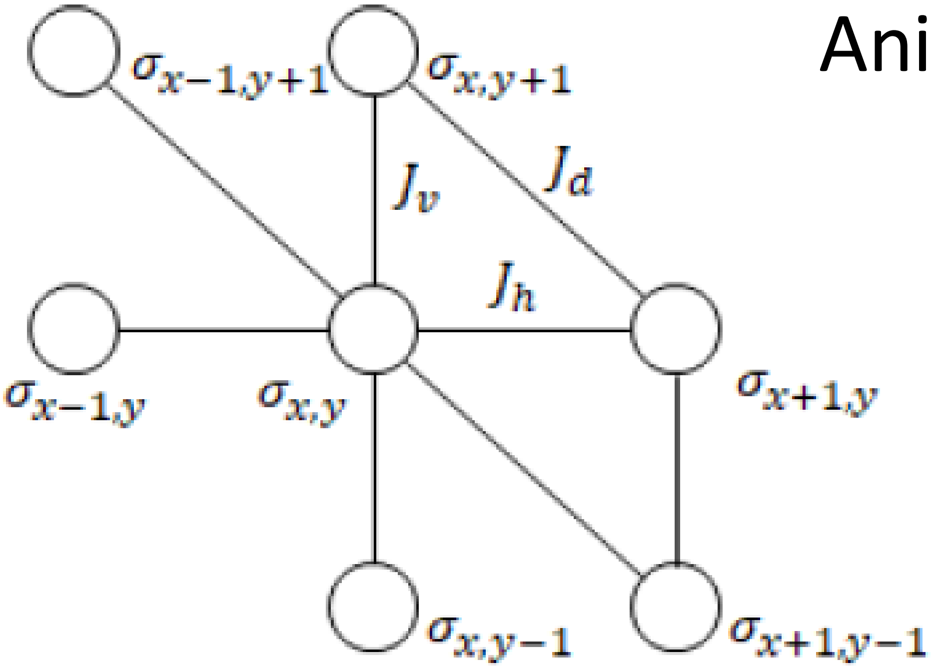
Моделирование образцов → Конфигурация спинов → Нейронная сеть → Бинарная классификацияа $f_i(T)$

T

$$P(T;L) = \frac{1}{N}\sum_{i=1}^{N} f_i(T;L)$$

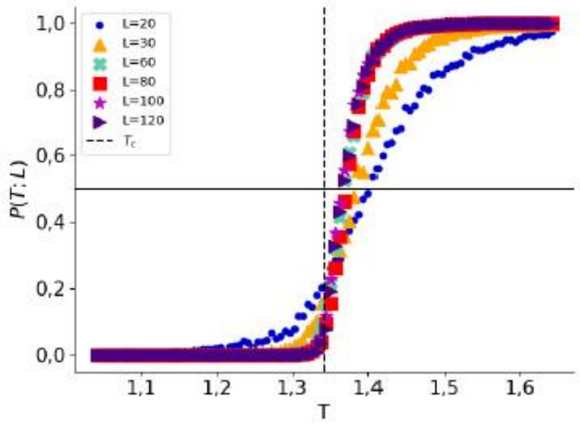
Anisotropy

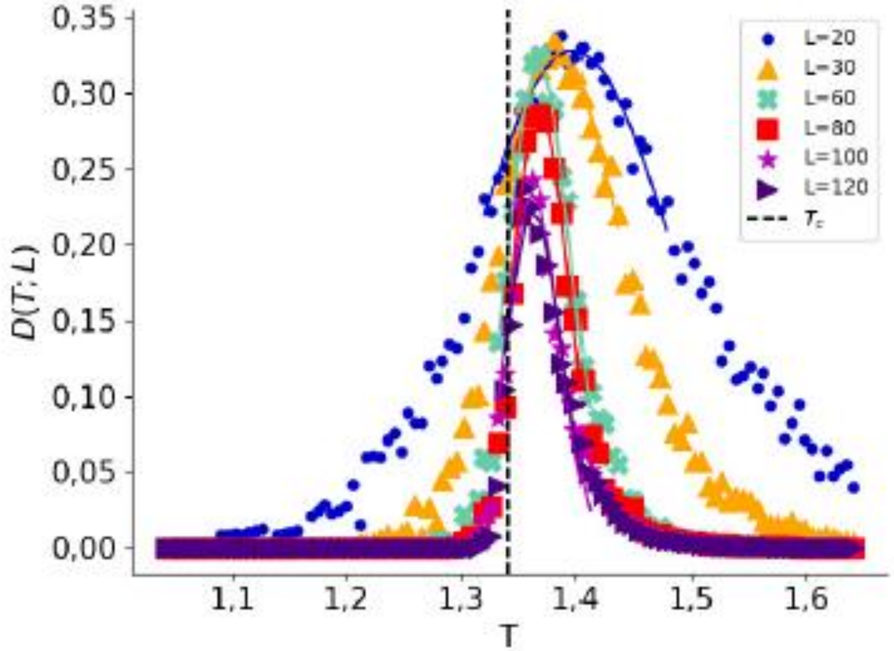
Houtappel, Physica **16**, 425 (1950).



$$\sinh\frac{2J_v}{k_BT_c}\,\sinh\frac{2J_h}{k_BT_c}+\sinh\frac{2J_h}{k_BT_c}\,\sinh\frac{2J_d}{k_BT_c}+ +\sinh\frac{2J_d}{k_BT_c}\,\sinh\frac{2J_v}{k_BT_c}=1$$

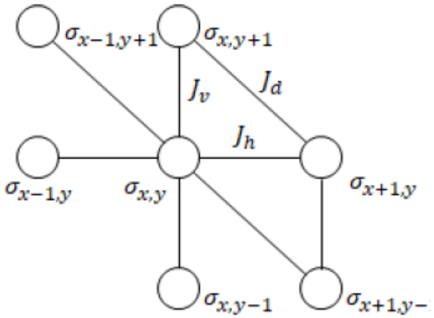
$$J_v+J_h>0,\ \ J_h+J_d>0,\ \ J_d+J_v>0$$

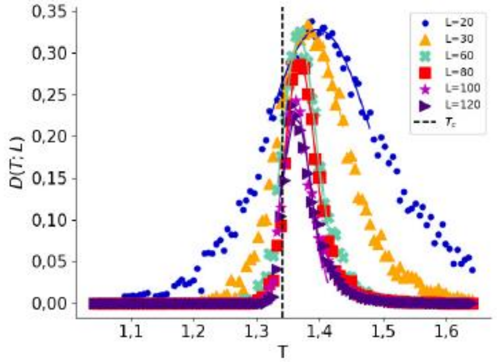


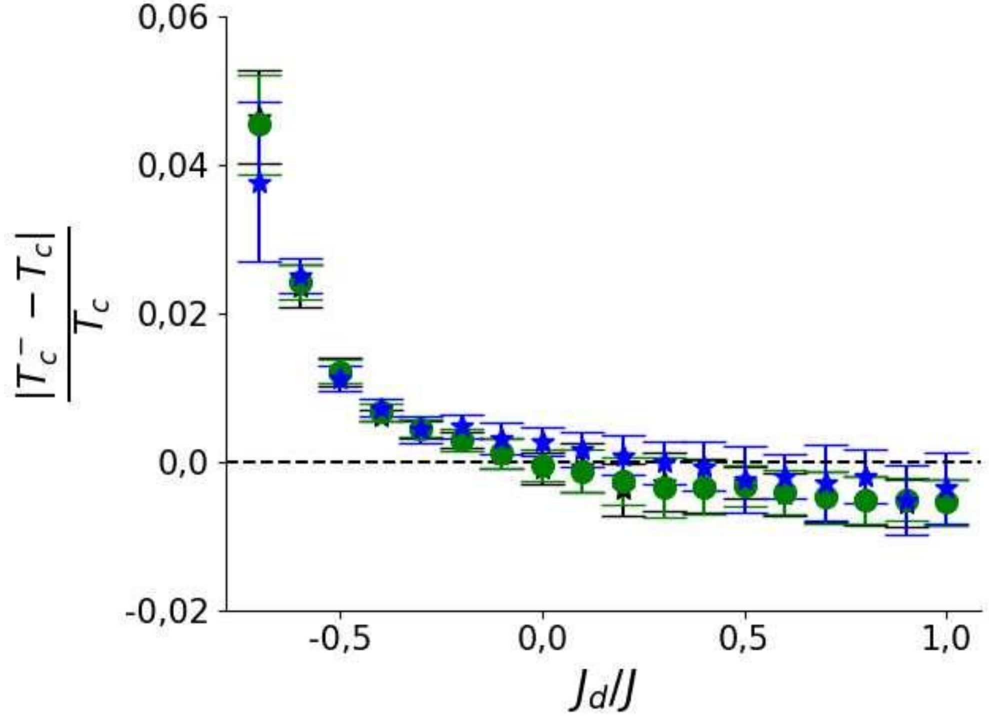


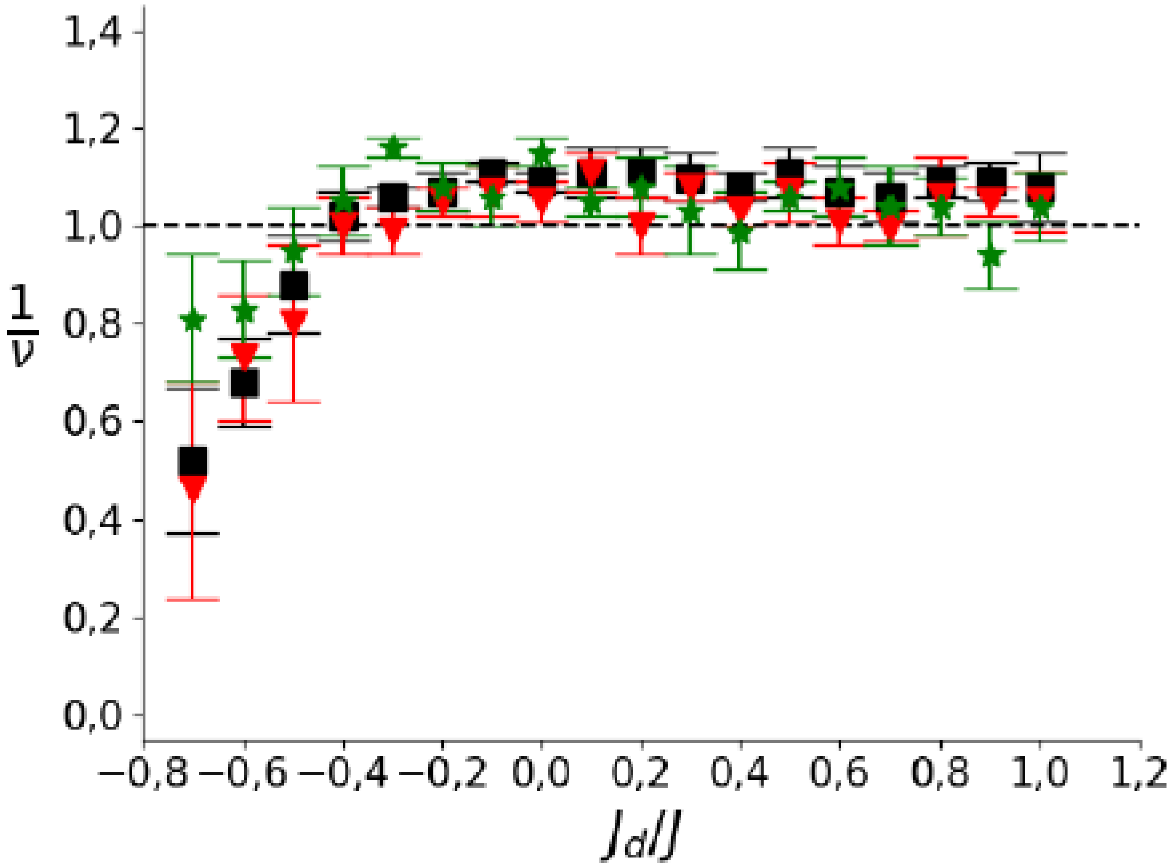
Sukhoverhova, LS: JETP Letters (202

Training – isotropic Ising model
Testing - anisotropic model

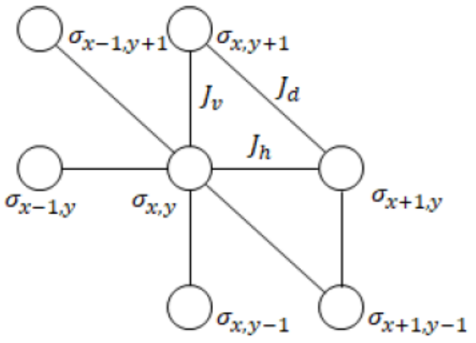


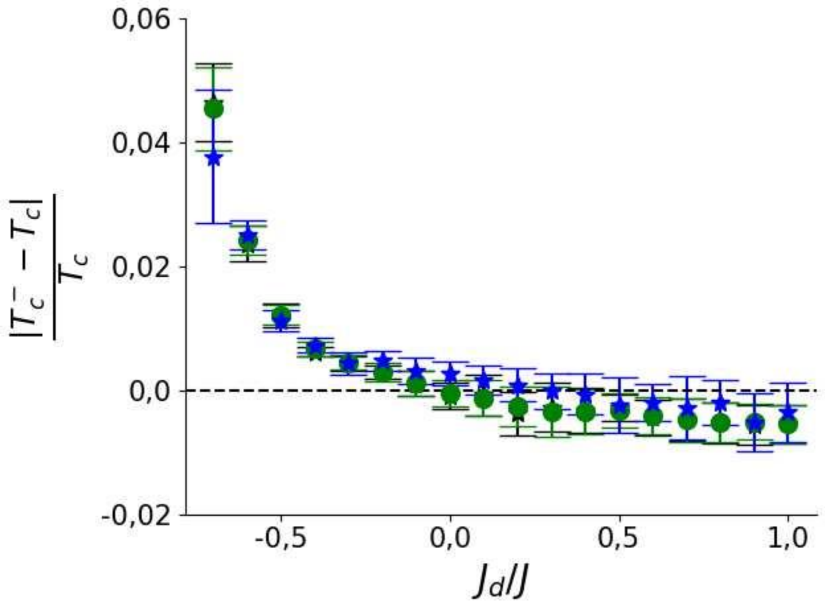


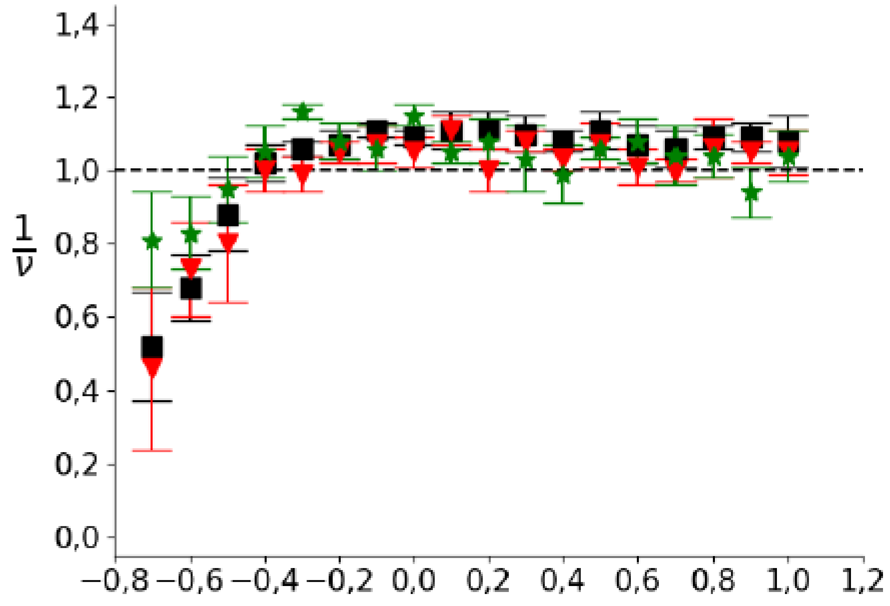




Sukhoverhova, LS: JETP Letters (2024)

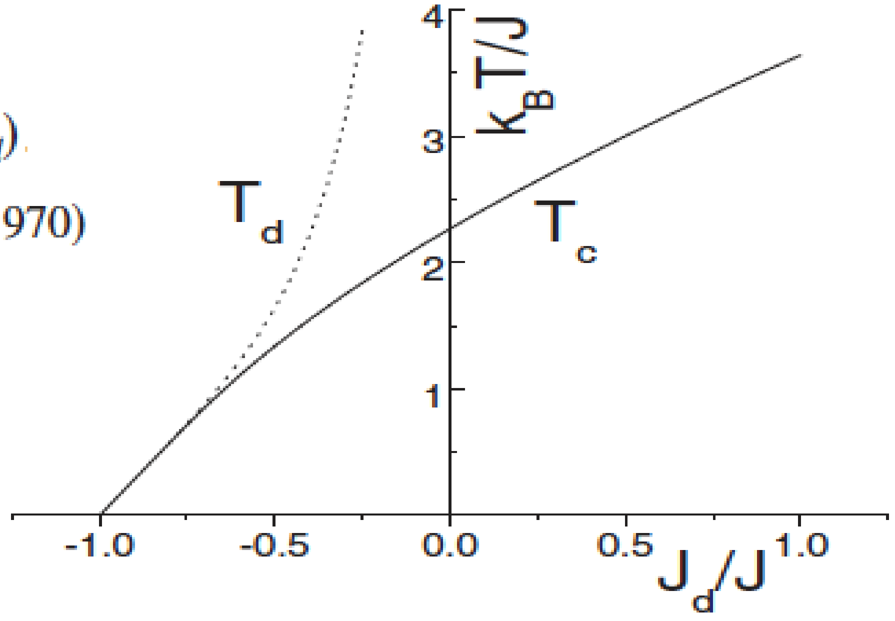






$$\cosh(2J/k_BT_d) = \exp(-2J_d/k_BT_d)$$

Stephenson, Phys. Rev. B 1, 4405 (1970)



Oscillatory decay of the spin-spin correlation function above T_d

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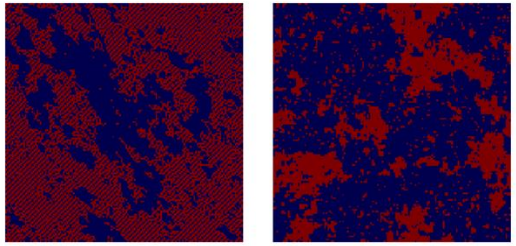


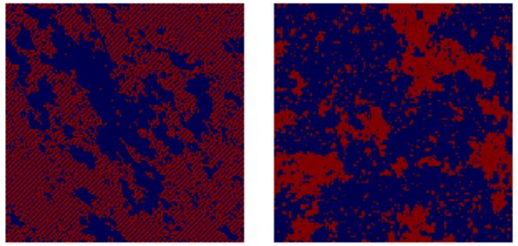
Обучение на одной модели

Моделирование образцов → Конфигурация спинов → Нейронная сеть

FM/PM

Бинарная классификация

Transfer learning between universality classes



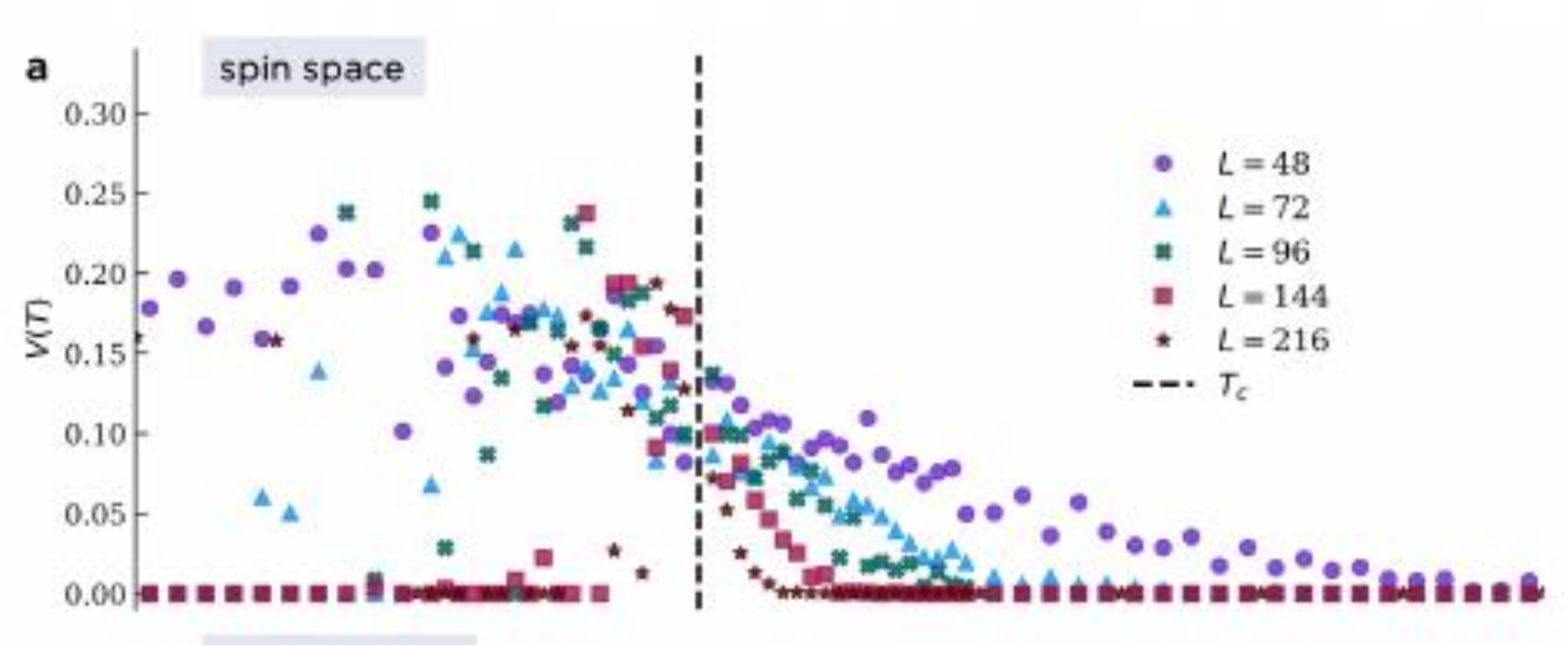
Тестирование модели из другого класса универсальности

Моделирование образцов → Конфигурация спинов → Нейронная сеть → Бинарная классификацияа $f_i(T)$

T

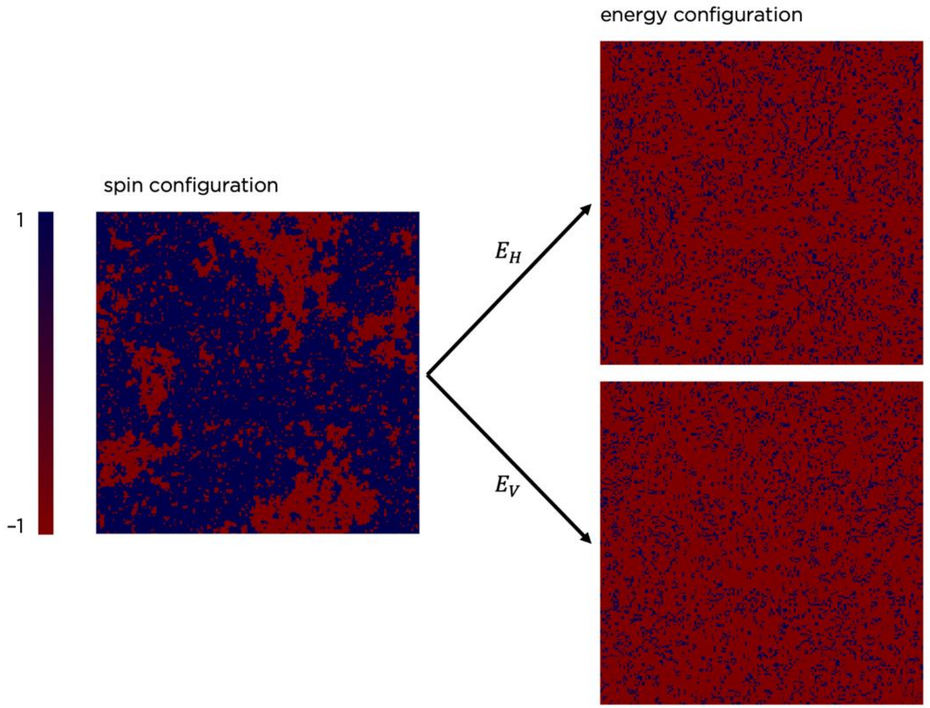
$$P(T;L) = \frac{1}{N}\sum_{i=1}^{N} f_i(T;L)$$

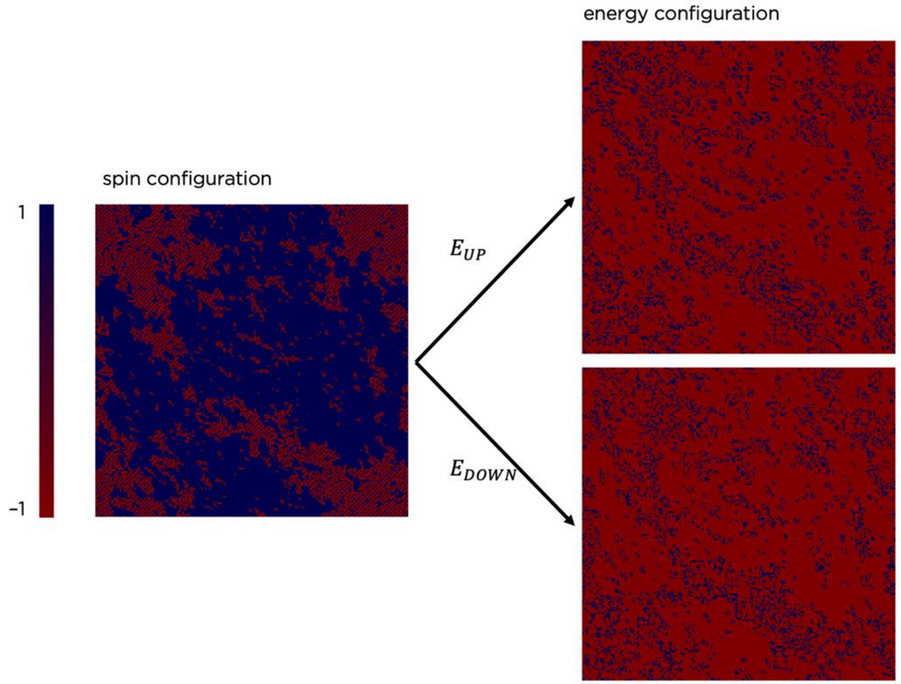
Inter-domain training/testing – different universality classes
Обучение – модель Изинга, тестирование – модель Бакстера-Ву



Chertenkov, LS: PhysRev (2024)

Преобразование спиновых конфигураций в конфигурации энергий





$$\mathcal{H}_{ising} = -J \sum_{(i,j)} [\sigma_{i,j}\sigma_{i+1,j} + \sigma_{i,j}\sigma_{i,j+1}]$$

$$\mathcal{H}_{bw} = -J \sum_{(i,j)} [\sigma_{i,j}\sigma_{i+1,j}\sigma_{i+1,j+1} + \sigma_{i,j}\sigma_{i,j+1}\sigma_{i+1,j+1}]$$

Chertenkov, LS: PhysRev (2024)

Обучение – модель Бакстера-Ву, тестирование – модель Изинга

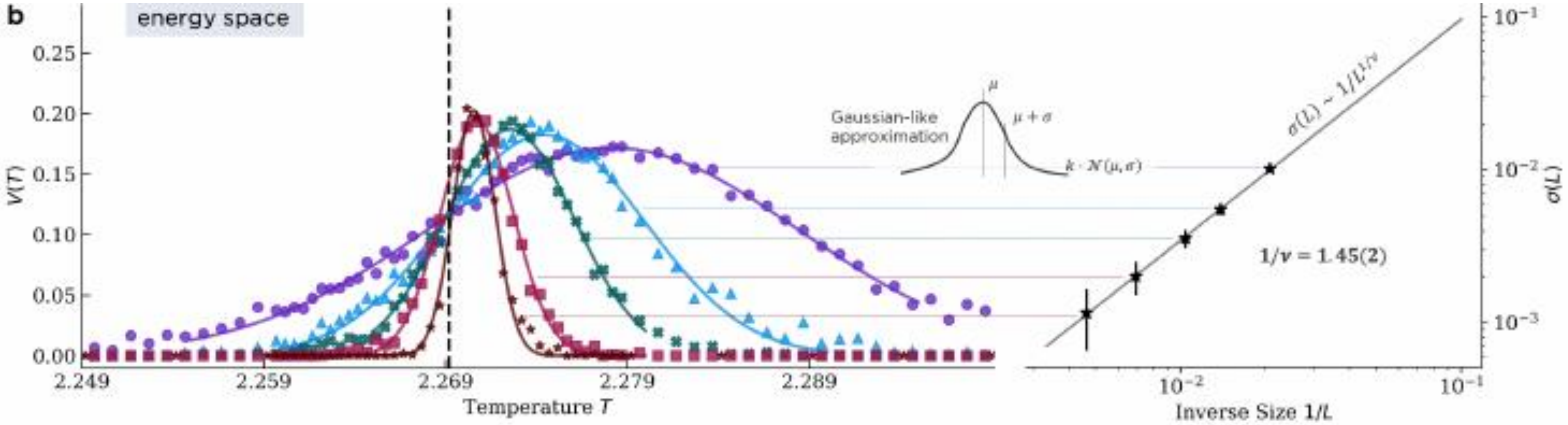
IS@IS	$1/\nu_\sigma$	$1/\nu_{\sigma-}$	$1/\nu_{\sigma+}$
CNN	1.12(3)	1.15(5)	1.07(2)
ResNet-10	1.15(3)	1.17(6)	1.09(11)

IS@BW	$1/\nu_\sigma$	$1/\nu_{\sigma-}$	$1/\nu_{\sigma+}$
CNN	1.16(5)	1.31(8)	0.98(1)
ResNet-10	0.85(6)	1.13(11)	0.78(15)

NN	T^*, IS@BW	Δ/ϵ	T^*, BW@IS	Δ/ϵ
CNN	2.226(24)	1.8	2.2694(2)	1
ResNet-10	2.214(21)	2.6	2.2686(5)	1.2

Chertenkov, LS: PhysRev (2024)

Обучение – модель Изинга, тестирование – модель Бакстера-Ву



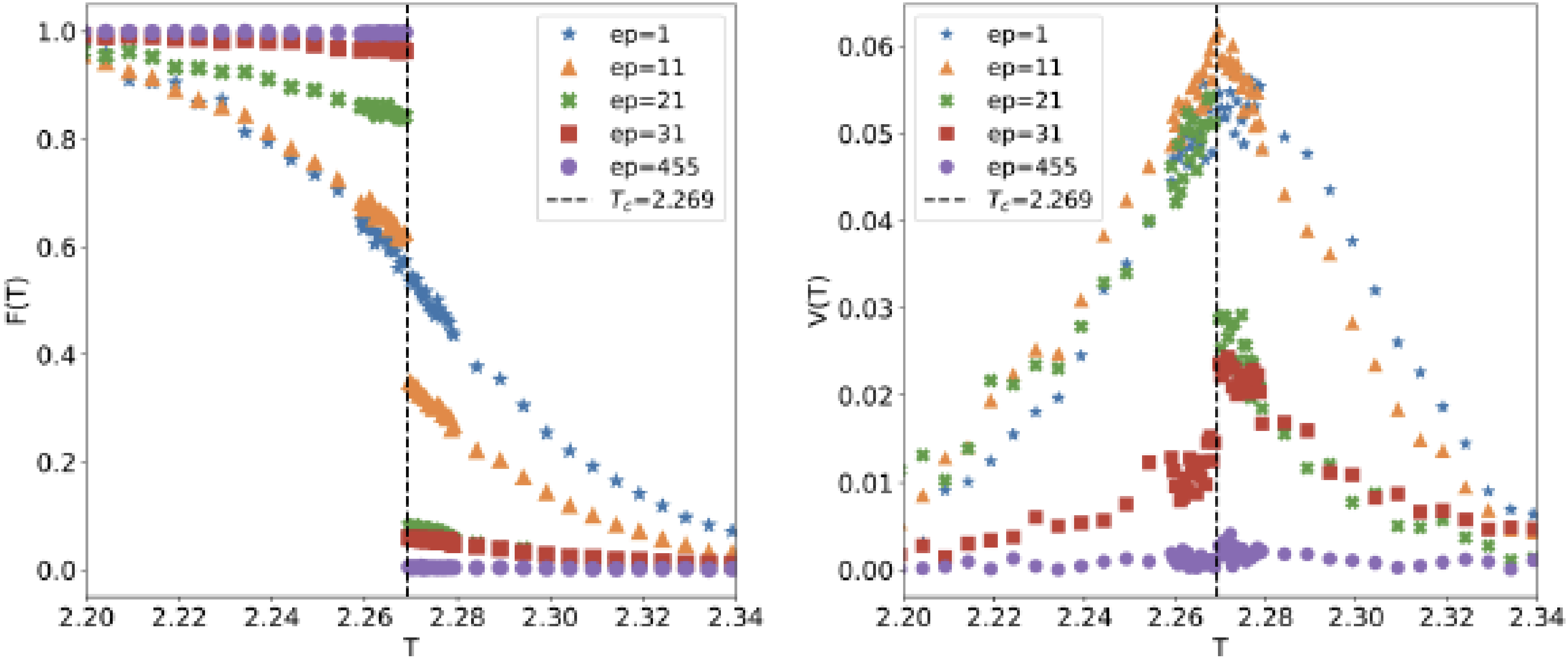
BW@BW	$1/\nu_\sigma$	$1/\nu_{\sigma^-}$	$1/\nu_{\sigma^+}$
CNN	1.48(5)	1.61(10)	1.52(3)
ResNet-10	1.50(7)	1.62(17)	1.52(4)
BW@IS	$1/\nu_\sigma$	$1/\nu_{\sigma^-}$	$1/\nu_{\sigma^+}$
CNN	1.45(2)	1.51(2)	1.42(6)
ResNet-10	1.45(3)	1.45(10)	1.47(4)

Chertenkov, LS: PhysRev (2024)

Conclusion

1. Finite-size scaling of the variation of the output function allows us to determine the correlation length exponent and the critical temperature
2. Diagonal anisotropy does not change the estimates of the correlation length exponent and critical temperature over a wide range of anisotropy ratio.
3. Deviation associated with a region on the phase diagram with oscillatory decay of the spin-spin correlation function.
4. Transfer-learning of models of different universality class is possible with appropriate choice of training/testing domain.

Поддержано грантом РНФ 22-21-00259


F(T)
1.0
0.8
0.6
0.4
0.2
0.0
2.20 2.22 2.24 2.26 2.28 2.30 2.32 2.34
T
ep=1
ep=11
ep=21
ep=31
ep=455
T_c=2.269
V(T)
0.06
0.05
0.04
0.03
0.02
0.01
0.00
2.20 2.22 2.24 2.26 2.28 2.30 2.32 2.34
T
ep=1
ep=11
ep=21
ep=31
ep=455
T_c=2.269